

2-Chloronaphthalene
91-58-7 | DTXSID8023971

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.91	1.08	0.91	1.08	0.92	1.00

Model Results

Predicted value: 1.84e-02 mmHg

Global applicability domain: Inside

Local applicability domain index: 7.49e-01

Confidence level: 7.19e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>2-Methylnaphthalene</div> <div>Measured: 1.22e-02</div> <div>Predicted: 2.48e-02</div>	<div>Image not found</div> <div>1-Methylnaphthalene</div> <div>Measured: 2.90e-02</div> <div>Predicted: 2.13e-02</div>	<div>Image not found</div> <div>1-Methoxy-2-nitrobenzene</div> <div>Measured: 8.93e-03</div> <div>Predicted: 6.33e-03</div>
<div>Image not found</div> <div>Benzoic acid, 2,4-dimethoxy-</div> <div>Measured: 5.50e-02</div> <div>Predicted: 1.58e-05</div>	<div>Image not found</div> <div>1,2-Dinitrobenzene</div> <div>Measured: 1.31e-02</div> <div>Predicted: 1.59e-04</div>	